

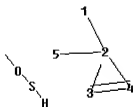
# STN Search 10580317

=>

Uploading C:\Program Files\STNEXP\Queries\10580317\str#1.str

AK

6



chain nodes :

1 5 6 7 8 9 10

ring nodes :

2 3 4

chain bonds :

1-2 2-5 7-8 8-9 9-10

ring bonds :

2-3 2-4 3-4

exact/norm bonds :

2-3 2-4 3-4 7-8 8-9

exact bonds :

1-2 2-5 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:CLASS

Generic attributes :

1:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

6:

Number of Carbon Atoms : 7 or more

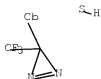
L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

Id



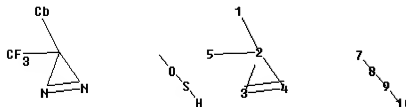
Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\STNEXP\Queries\10580317\str#1.str

AK

6



chain nodes :

1 5 6 7 8 9 10

ring nodes :

2 3 4

chain bonds :

1-2 2-5 7-8 8-9 9-10

ring bonds :

2-3 2-4 3-4

exact/norm bonds :

2-3 2-4 3-4 7-8 8-9

exact bonds :

1-2 2-5 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS

Generic attributes :

1:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

6:

Number of Carbon Atoms : 7 or more

L4 STRUCTURE UPLOADED

=> s l4

SAMPLE SEARCH INITIATED 17:59:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 6785 TO ITERATE

29.5% PROCESSED 2000 ITERATIONS 0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 130761 TO 140639  
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4

SAMPLE SEARCH INITIATED 17:59:47 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 6785 TO ITERATE

29.5% PROCESSED 2000 ITERATIONS 0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 130761 TO 140639  
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L4

=> s l4 full

FULL SEARCH INITIATED 18:00:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 136843 TO ITERATE

100.0% PROCESSED 136843 ITERATIONS 13 ANSWERS  
SEARCH TIME: 00.00.14

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:end

=> s l7

L8 12 L7

=> d ibib abs hitstr 1-12

L8 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2008:1130736 CAPLUS Full-text  
DOCUMENT NUMBER: 150:347185  
TITLE: Improvement of photoaffinity SPR imaging platform and  
determination of the binding site of p62/SQSTM1 to p38  
MAP kinase  
AUTHOR(S): Saito, Akiko; Kawai, Kayoko; Takayama, Hiroshi; Sudo,  
Tatsuhiko; Osada, Hiroyuki  
CORPORATE SOURCE: Antibiotics Laboratory Chemical Biology Department  
Advanced Research Institute, RIKEN, 2-1 Hirosawa,  
Wako, Saitama, 351-0198, Japan  
SOURCE: Chemistry--An Asian Journal (2008), 3(8-9), 1607-1612  
CODEN: CAAJBI; ISSN: 1861-4728  
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 150:347185

AB P38 mitogen-activated protein kinase (MAPK) is a member of the serine/threonine kinases and is activated in response to stress stimuli, such as cytokines, UV irradiation, heat shock, and osmotic shock. We revealed in a previous report that p62/SQSTM1, known to participate in proteasomal or autophagosomal protein degradation and cytokine receptor signal transduction pathways, binds to p38 to regulate specifically. Herein, we describe the improvement of the photoaffinity-thiol linker of our SPR imaging platform, which enabled us to determine the binding site of p62 to p38. SPR imaging expts. using a new photoaffinity linker 2 to immobilize the peptides derived from p62 on gold substrate indicate that the domain comprising amino acids 164-190 of p62 binds to p38 directly. These SPR anal. data and empirical biol. data reveal that the binding site of p62 to p38 is the domain corresponding to 173-182.

IT 882522-65-8P 1134189-75-5P 1134189-76-6P  
 1134189-77-7P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

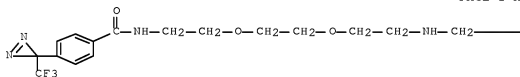
(improvement of photoaffinity SPR imaging platform and determination of binding

site of p62/SQSTM1 to p38 MAP kinase using)

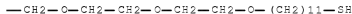
RN 882522-65-8 CAPLUS

CN Benzamide, N-(29-mercapto-3,6,12,15,18-pentaoxa-9-azanonacos-1-yl)-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)

PAGE 1-A



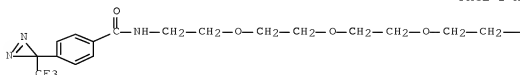
PAGE 1-B



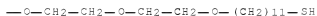
RN 1134189-75-5 CAPLUS

CN Benzamide, N-(29-mercapto-3,6,9,12,15,18-hexaoxanonacos-1-yl)-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)

PAGE 1-A



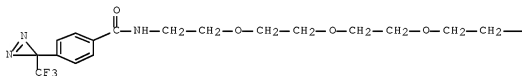
PAGE 1-B



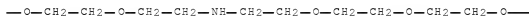
RN 1134189-76-6 CAPLUS

CN Benzamide, N-(38-mercapto-3,6,9,12,15,21,24,27-octa-oxa-18-aza-octatriacont-1-yl)-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



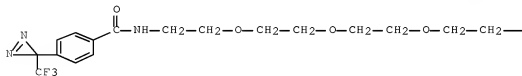
PAGE 1-C



RN 1134189-77-7 CAPLUS

CN Benzamide, N-(38-mercapto-3,6,9,12,15,18,21,24,27-nona-oxa-octatriacont-1-yl)-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)

PAGE 1-A



—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—

—(CH<sub>2</sub>)<sub>11</sub>—SH

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)  
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2006:386326 CAPLUS Full-text  
DOCUMENT NUMBER: 144:407736  
TITLE: Biomolecule interaction label-free observation method  
using drug-array produced by photoreaction  
INVENTOR(S): Kanoh, Naoki; Osada, Hiroyuki; Kyo, Motoki  
PATENT ASSIGNEE(S): Riken Corp., Japan; Toyo Boseki Kabushiki Kaisha  
SOURCE: PCT Int. Appl., 32 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006043461	A1	20060427	WO 2005-JP18841	20051013
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM JP 2006118920 A 20060511 JP 2004-305605 20041020 EP 1811301 A1 20070725 EP 2005-793178 20051013 R: DE, FR, GB US 20080124809 A1 20080529 US 2007-665636 20070418 PRIORITY APPLN. INFO.: JP 2004-305605 A 20041020 WO 2005-JP18841 W 20051013				

AB A biomol. interaction observation method is provided, with which the  
interaction of a substance (e.g., drug) immobilized on a metal baseplate with a  
biomol. (e.g., protein) is observed in a label-free fashion by a surface  
plasmon resonance method or a surface plasmon resonance imaging method. The

method is characterized in that the substance is immobilized on the metal baseplate by a covalent bond through a photoreaction.

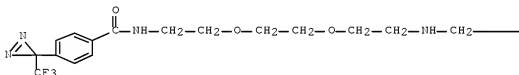
IT 882522-65-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(biomol. interaction label-free observation method using drug-array produced by photoreaction)

RN 882522-65-8 CAPLUS

CN Benzamide, N-(29-mercapto-3,6,12,15,18-pentaoxa-9-azanonacos-1-yl)-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—(CH<sub>2</sub>)<sub>11</sub>—SH

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2006:174155 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:384441

TITLE: Study of the Interaction between Actin and Antitumor Substance Aplyronine A with a Novel Fluorescent Photoaffinity Probe

AUTHOR(S): Kuroda, Takeshi; Suenaga, Kiyotake; Sakakura, Akira; Handa, Tomohisa; Okamoto, Kazuhito; Kigoshi, Hideo

CORPORATE SOURCE: Department of Chemistry, University of Tsukuba, Tsukuba, Ibaraki, 305-8571, Japan

SOURCE: Bioconjugate Chemistry (2006), 17(2), 524-529  
CODEN: BCCHE; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:384441

AB The interaction between actin and aplyronine A, a potent antitumor and actin-depolym. substance of marine origin, was investigated by photoaffinity labeling expts. Photoaffinity probes consisting of a side-chain portion of aplyronine A as a ligand, a diazidine moiety as a photoaffinity group, and a fluorophore as a detecting group were synthesized. Photolabeling expts. between actin and the probe were carried out. Actin was successfully photolabeled by the fluorescent probe and visualized clearly. The present results provide the first chemical evidence for the direct interaction between actin and the side-chain portion of aplyronine A.

IT 883449-34-1P

RL: ANT (Analyte); SPN (Synthetic preparation); ANST (Analytical study);

PREP (Preparation)

(interaction between actin and antitumor substance aplyronine A with novel fluorescent photoaffinity probe)

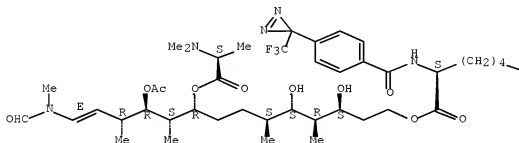
RN 883449-34-1 CAPLUS

CN L-Lysine, N6-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9']-[9H]xanthen)-5-yl]amino]thioxomethyl]-N2-[4-[3-(trifluoromethyl)-3H-diazirin-3-yl]benzoyl]-, (3S,4R,5S,6S,9R,10S,11R,12R,13E)-11-(acetyloxy)-9-[ (2S)-2-(dimethylamino)-1-oxopropoxy]-14-(formylmethylamino)-3,5-dihydroxy-4,6,10,12-tetramethyl-13-tetradecen-1-yl ester (CA INDEX NAME)

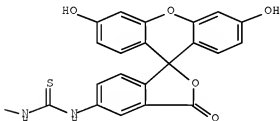
Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2006:152860 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:365629

TITLE: SPR Imaging of Photo-Cross-Linked Small-Molecule Arrays on Gold

AUTHOR(S): Kanoh, Naoki; Kyo, Motoki; Inamori, Kazuki; Ando, Ami; Asami, Aya; Nakao, Aiko; Osada, Hiroyuki



CORPORATE SOURCE: Antibiotics Laboratory and Beam Application Team,  
Discovery Research Institute, Saitama, 351-0198, Japan  
SOURCE: Analytical Chemistry (2006), 78(7), 2226-2230  
CODEN: ANCHAM; ISSN: 0003-2700  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Identification of small-mol. ligands for a protein of interest can facilitate the anal. of the protein's functions in biol. systems. Small-mol. microarrays have allowed for rapid detection of such ligand-protein interactions in a high-throughput manner, although a label on a protein is needed to observe these interactions. By combining SPR imaging technol. with the authors' recently developed photo-cross-linked small-mol. array platform, the authors developed a novel platform that allows in situ observation of interactions between photo-cross-linked small mols. on gold surfaces and nonlabeled proteins in solution. As a proof-of-concept study, the authors selected six small mols. whose antibodies and binding proteins are known and com. available. Addnl., interactions of 8 estrogenic and androgenic substances with estrogen receptor  $\alpha$  were observed using this platform.

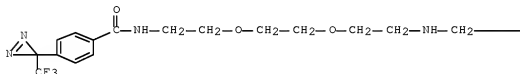
IT 882522-65-8P  
RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); DEV (Device component use); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)

(photocrosslinker; surface plasmon resonance imaging of photo-cross-linked small-mol. arrays on gold)

RN 882522-65-8 CAPLUS

CN Benzamide, N-(29-mercapto-3,6,12,15,18-pentaoxa-9-azanonacos-1-yl)-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—(CH<sub>2</sub>)<sub>11</sub>—SH

OS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)  
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2009 ACS ON STN  
ACCESSION NUMBER: 2004:69457 CAPLUS Full-text  
DOCUMENT NUMBER: 140:304077  
TITLE: On penicillin-binding protein 1b affinity-labeling reagents

AUTHOR(S): Volke, Daniela; Daghigh, Mohammed; Hennig, Lothar; Findeisen, Matthias; Giesa, Sabine; Oehme, Ramona; Welzel, Peter

CORPORATE SOURCE: Universitaet Leipzig, Fakultae fuer Chemie und Mineralogie, Leipzig, D-04103, Germany

SOURCE: Helvetica Chimica Acta (2003), 86(12), 4214-4232  
CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:304077

AB The synthesis of some 3-aryl-3-(trifluoromethyl)3H-diazirine and benzophenone-based photoaffinity labels is reported. The photolabile group is bound to a scaffold that also accommodates functional groups to which an indicator unit (biotin) and the bioactive ligand can be attached orthogonally. To three of the labels, moenomycin was conjugated with the aim to provide tools for the identification of the moenomycin binding site within the transglycosylase domain of the enzyme PBP 1b. Some preliminary photoaffinity-labeling expts. were carried out.

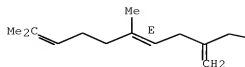
IT 473912-44-6P  
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(synthesis of diazirine and benzophenone-based moenomycin-derived photoaffinity labels for identification of moenomycin A binding site within transglycosylase domain of enzyme PBP 1b)

RN 473912-44-6 CAPLUS

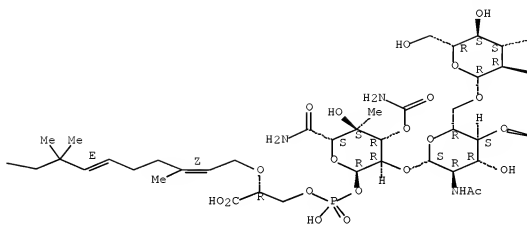
CN  $\alpha$ -D-Glucopyranuronamide, O-(5R)-5-C-[3-(3-carboxy-1-oxopropyl)-1-[3-[12-[4-[(3R)-24-[3aS,4S,6aR]-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-3-[[[[2-[3-nitro-5-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenoxy]ethoxy]carbonyl]amino]methyl]-1,4,20-trioxo-2,9,12,15-tetraoxa-5,19-diazatetracos-1-yl]phenyl]amino]-1-oxo-12-thioxo-5,8-dioxo-2,11-diazadodec-1-yl]-4-nitrophenyl]-1H-1,2,4-triazol-5-yl]- $\alpha$ -L-arabinopyranosyl-(1 $\rightarrow$ 4)-O-2-(acetylamino)-2,6-dideoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-[ $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)]-O-2-(acetylamino)-2-deoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)-4-C-methyl-, 3-carbamate 1-[ (2R)-2-carboxy-2-[[ (2Z,6E,13E)-3,8,8,14,18-pentamethyl-11-methylene-2,6,13,17-nonadecatetraenyl]oxy]ethyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

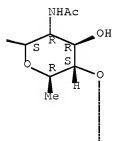
PAGE 1-A



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PAGE 1-C





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OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
(7 CITINGS)  
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2002:548920 CAPLUS Full-text

DOCUMENT NUMBER: 137:337550

TITLE: Tetrafunctional photoaffinity labels based on  
Nakanishi's m-nitroalkoxy-substituted  
phenyltrifluoromethyldiazirine

AUTHOR(S): Daghigh, Mohammed; Hennig, Lothar; Findeisen,  
Matthias; Giesa, Sabine; Schumer, Frank; Hennig,  
Horst; Beck-Sickinger, Annette G.; Welzel, Peter

CORPORATE SOURCE: Institut fur Organische Chemie Universitat Leipzig,  
Leipzig, 04103, Germany

SOURCE: Angewandte Chemie, International Edition (2002),  
41(13), 2293-2297

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:337550

AB Two generally applicable reagents for photoaffinity probes have been developed. They contain an m-nitrophenyl ether function with a trifluoromethyldiazirine side chain (photophore group), as well as a biotin tag for the identification of labeled proteins or peptides and either a free hydroxy or a squaramide group for the attachment of any suitably functionalized ligand which directs the reagent to the binding site of the target mol.

IT 808108-93-2P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);  
BIOL (Biological study); PREP (Preparation)

(preparation of tetrafunctional photoaffinity labels based on  
m-nitroalkoxy-substituted phenyl(trifluoromethyl)diazirine, their  
coupling with moenomycin derivs., and antibiotic activity of the  
labeled moenomycins)

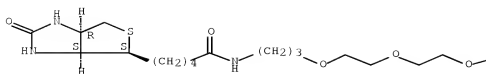
RN 808108-93-2 CAPLUS

CN  $\alpha$ -D-Glucopyranuronamide, O-(5R)-5-C-[3-(3-carboxy-1-oxopropyl)-1-[3-[15-[[4-[(3R)-24-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-3-[[[2-[3-nitro-5-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenoxy]ethoxy]carbonyl]amino]methyl]-1,4,20-trioxo-2,9,12,15-tetraoxa-5,19-diazatetracos-1-yl]phenyl]amino]-1-oxo-15-thioxo-5,8,11-trioxo-2,14-diazapentadec-1-yl]-4-nitrophenyl]-1H-1,2,4-triazol-5-yl]- $\alpha$ -L-arabinopyranosyl-(1 $\rightarrow$ 4)-O-2-(acetylamino)-2,6-dideoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-[ $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)]-O-2-(acetylamino)-2-deoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)-4-C-methyl-, 3-carbamate 1-[1(2R)-2-carboxy-2-[[[(2Z,6E,13E)-3,8,8,14,18-pentamethyl-11-methylene-2,6,13,17-nonadecatetraenyl]oxy]ethyl hydrogen phosphate] (9CI) (CA INDEX NAME)

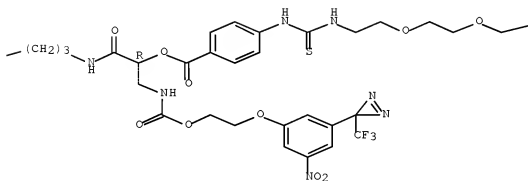
Absolute stereochemistry.

Double bond geometry as shown.

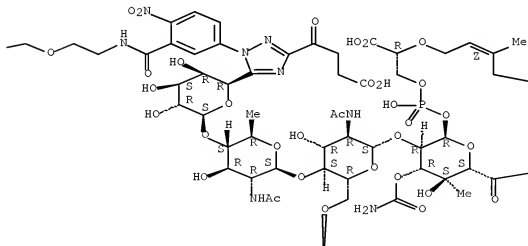
PAGE 1-A

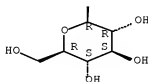
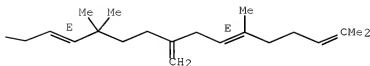


PAGE 1-B



PAGE 1-C





OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS  
RECORD (13 CITINGS)  
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:517309 CAPLUS Full-text

DOCUMENT NUMBER: 137:291198

TITLE: Isoserine-based biotinylated photoaffinity probes that  
interact with penicillin-binding protein 1b

AUTHOR(S): Ruehl, Thomas; Volke, Daniela; Stembera, Katherina;  
Hatanaka, Yasumaru; Hennig, Horst; Schumer, Frank;  
Welzel, Peter

CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Leipzig,  
Leipzig, D-04103, Germany

SOURCE: Chemical Communications (Cambridge, United Kingdom)  
(2002), (15), 1630-1631

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The photolytic decomposition of trifunctional carbene generating photoaffinity  
probes in methanolic solution was studied, a cleavage reaction with butylamine  
in water, the conjugation with a ligand (moenomycin), and expts. that  
demonstrate that the fully armed probes interact with penicillin-binding  
protein 1b.

IT 468061-42-9P 468061-44-1P

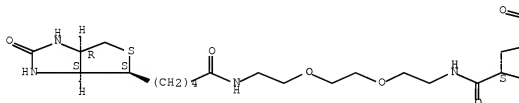
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation)  
(isoserine-based biotinylated photoaffinity probes that interact with  
penicillin-binding protein 1b)

RN 468061-42-9 CAPLUS

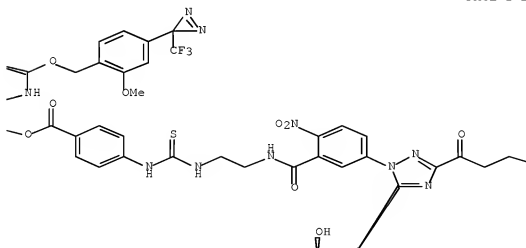
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4-yl]-3-[[[[2-methoxy-4-[3-(trifluoromethyl)-3H-diazirin-3-  
yl]phenyl]methoxy]carbonyl]amino]methyl]-1,4,15-trioxo-2,8,11-trioxa-5,14-  
diazanonadec-1-yl]phenyl]amino]thioxomethyl]amino]ethyl]amino]carbonyl]-4-  
nitrophenyl]-1H-1,2,4-triazol-5-yl]- $\alpha$ -L-arabinopyranosyl-  
(1 $\rightarrow$ 4)-O-2-(acetylamino)-2,6-dideoxy- $\beta$ -D-glucopyranosyl-  
(1 $\rightarrow$ 4)-O-[ $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)]-O-2-(acetylamino)-2-  
deoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)-4-C-methyl-, 3-carbamate  
1-[(2R)-2-carboxy-2-[[[(2Z,6E)-3,8,8,14,18-pentamethyl-11-methylene-  
2,6,13,17-nonadecatetraenyl]oxy]ethyl hydrogen phosphate] (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

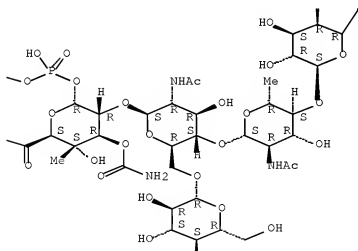
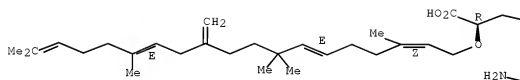
PAGE 1-A



PAGE 1-B







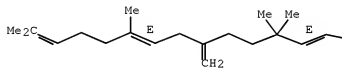


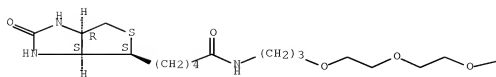
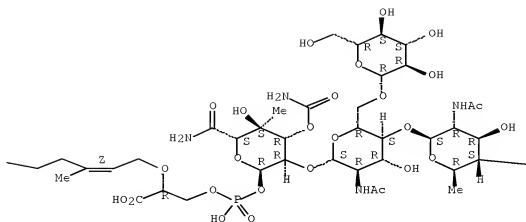
RN 468061-44-1 CAPLUS

CN  $\alpha$ -D-Glucopyranuronamide, O-(5R)-5-C-[3-(3-carboxy-1-oxopropyl)-1-[3-[[[2-[[[4-(3S)-24-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-3-[[[2-methoxy-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]methoxy]carbonyl]amino]methyl]-1,4,20-trioxo-2,9,12,15-tetraoxa-5,19-diazatetracos-1-yl]phenyl]amino]thioxomethyl]amino]ethyl]amino]carbon-yl]-4-nitrophenyl]-1H-1,2,4-triazol-5-yl]- $\alpha$ -L-arabinopyranosyl-(1 $\rightarrow$ 4)-O-2-(acetylamino)-2,6-dideoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-[ $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)]-O-2-(acetylamino)-2-deoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)-4-C-methyl-, 3-carbamate 1-[(2R)-2-carboxy-2-[[[(2Z,6E,13E)-3,8,8,14,18-pentamethyl-11-methylene-2,6,13,17-nonadecatetraenyl]oxy]ethyl hydrogen phosphate] (9CI) (CA INDEX NAME)

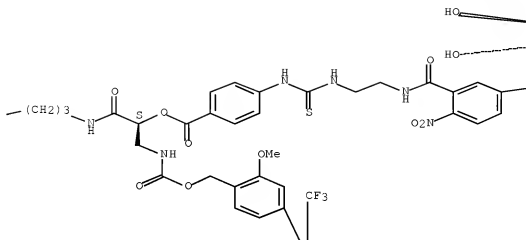
Absolute stereochemistry.

Double bond geometry as shown.

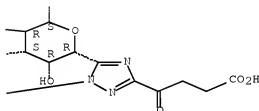




PAGE 2-B



PAGE 2-C



PAGE 3-B



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2001:905569 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 138:401975  
 TITLE: A trifunctional reagent for photoaffinity labeling.  
 [Erratum to document cited in CA133:208058]  
 AUTHOR(S): Ruhl, Thomas; Hennig, Lothar; Hatanaka, Yasumaru;

CORPORATE SOURCE: Burger, Klaus; Welzel, Peter  
 Institut für Organische Chemie, Universität Leipzig,  
 Leipzig, D-04103, Germany

SOURCE: Tetrahedron Letters (2001), 42(52), 9297  
 CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Compound 13 was synthesized starting from (S)-malic acid. In formulas 4, 5, and 6, the configuration at C-2 of the malic acid part and in formulas 8, 10, and 13 at C-2 of the isoserine unit must be reversed.

IT 290812-04-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of photolabel for affinity labeling of penicillin-binding protein (Erratum))

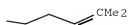
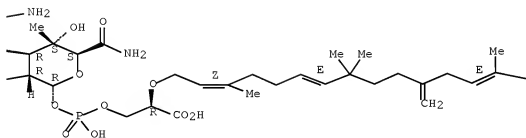
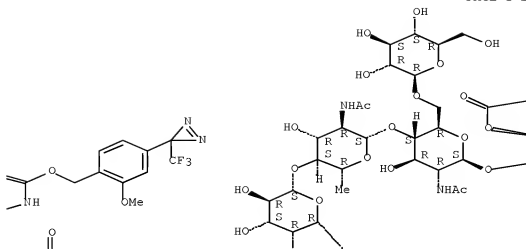
RN 290812-04-3 CAPLUS

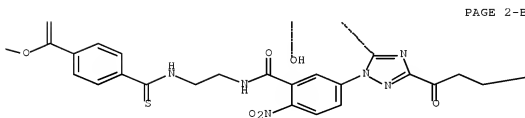
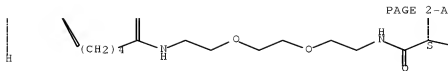
CN  $\alpha$ -D-Glucopyranuronamide, O-(5S)-5-C-[3-(3-carboxy-1-oxopropyl)-1-[3-[[[2-[[[4-(3R)-19-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-2-[[[2-methoxy-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]methoxy]carbonyl]amino]methyl]-1,4,15-trioxo-2,8,11-trioxa-5,14-diazanonadec-1-yl]phenyl]thioxomethyl]amino]ethyl]amino]carbonyl]-4-nitrophenyl]-1H-1,2,4-triazol-5-yl]- $\alpha$ -L-arabinopyranosyl-(1 $\rightarrow$ 4)-O-2-(acetylamino)-2,6-dideoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-[ $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)]-O-2-(acetylamino)-2-deoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)-4-C-methyl-, 3-carbamate 1-[(2R)-2-carboxy-2-[[[(2Z,6E,13E)-3,8,8,14,18-pentamethyl-11-methylene-2,6,13,17-nonadecatetraenyl]oxy]ethyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

PAGE 1-A







—CO<sub>2</sub>H

PAGE 2-C

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD  
(6 CITINGS)

L8 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:431259 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 133:208058

TITLE: A trifunctional reagent for photoaffinity labeling  
AUTHOR(S): Ruhl, Thomas; Hennig, Lothar; Hatanaka, Yasumaru;  
Burger, Klaus; Welzel, Peter

CORPORATE SOURCE: Universitat Leipzig, Institut fur Organische Chemie,  
Leipzig, D-04103, Germany

SOURCE: Tetrahedron Letters (2000), 41(23), 4555-4558

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:208058

AB A photolabel, a biotin tag, and a moenomycin ligand were attached orthogonally to the 3 functional groups of isoserine to provide a compound (I) that is to

be used in affinity labeling of penicillin-binding protein. The urethane group in I is cleaved with BuNH<sub>2</sub> in MeOH or H<sub>2</sub>O.

IT 290812-04-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of photolabel for affinity labeling of penicillin-binding protein)

RN 290812-04-3 CAPLUS

CN  $\alpha$ -D-Glucopyranuronamide, O-(5S)-5-C-[3-(3-carboxy-1-oxopropyl)-1-[3-[[[2-[[[4-[(3R)-19-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-2-[[[2-methoxy-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]methoxy]carbonyl]amino]methyl]-1,4,15-trioxo-2,8,11-trioxa-5,14-diazanonadec-1-yl]phenyl]thioxomethyl]amino]ethyl]amino]carbonyl]-4-nitrophenyl]-1H-1,2,4-triazol-5-yl]- $\alpha$ -L-arabinopyranosyl-(1 $\rightarrow$ 4)-O-2-(acetylamino)-2,6-dideoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-[ $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)]-O-2-(acetylamino)-2-deoxy- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)-4-C-methyl-, 3-carbamate 1-[(2R)-2-carboxy-2-[[[(2Z,6E,13E)-3,8,8,14,18-pentamethyl-11-methylene-2,6,13,17-nonadecatetraenyl]oxy]ethyl hydrogen phosphate] (9CI) (CA INDEX NAME)

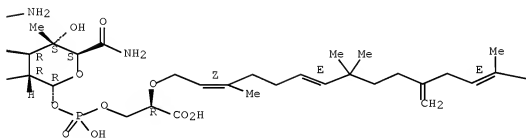
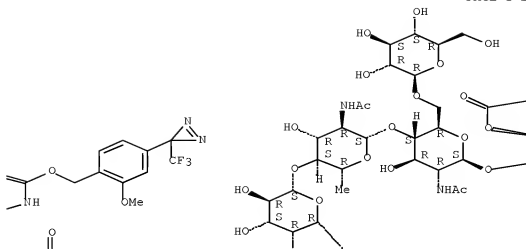
Absolute stereochemistry.

Double bond geometry as shown.

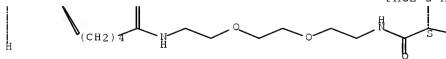
PAGE 1-A



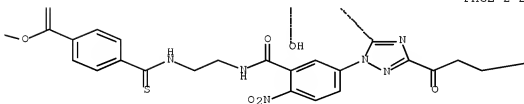




PAGE 2-A



PAGE 2-B



PAGE 2-C



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OS.CITING REF COUNT:      16   THERE ARE 16 CAPLUS RECORDS THAT CITE THIS
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REFERENCE COUNT:          13   THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
                             RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L8 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1996:625294 CAPLUS Full-text  
 DOCUMENT NUMBER: 125:242357  
 ORIGINAL REFERENCE NO.: 125:45169a,45172a  
 TITLE: Hydrophobic modified matrix surface for immobilization  
 of proteins and lipids  
 INVENTOR(S): Stein, Thomas  
 PATENT ASSIGNEE(S): Max-Planck-Gesellschaft Zur Foerderung Der  
 Wissenschaften EV, Germany  
 SOURCE: Ger., 8 pp.  
 CODEN: GWXXAW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

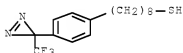
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4436173	C1	19960905	DE 1994-4436173	19941010
PRIORITY APPLN. INFO.:			DE 1994-4436173	19941010

AB The invention concerns. the modification of hydrophilic matrix surfaces with C4-12 chains or cycloaliph. or cycloarom. systems to produce hydrophobic surfaces on which lipids or proteins can be immobilized under gentle conditions. In an example, an 8 mm + 8 mm + 100 nm carboxymethyl dextran surface of a CM5 biosensor chip (Pharmacia) was activated and then modified with the photoactivatable crosslinker perfluorophenylamine (PFFA) using a hexyl spacer. Then a lipid-anchored cell adhesion mol. was covalently bound to the PFFA. The method also can be used with gel materials, e.g., dextran, cellulose, and agarose.

IT 182218-81-1  
 RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)  
 (hydrophobic modified matrixes for immobilization of proteins and lipids)

RN 182218-81-1 CAPLUS

CN Benzeneoctanethiol, 4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)  
 REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:465978 CAPLUS Full-text

DOCUMENT NUMBER: 117:65978

ORIGINAL REFERENCE NO.: 117:11519a,11522a

TITLE: Light-induced coupling of aqueous-soluble proteins to liposomes formed from carbene-generating phospholipids

AUTHOR(S): Saenger, Michael; Borle, Francois; Heller, Manfred; Sigrist, Hans

CORPORATE SOURCE: Inst. Biochem., Univ. Berne, Bern, CH-3012, Switz.

SOURCE: Bioconjugate Chemistry (1992), 3(4), 308-14

CODEN: BCCHE5; ISSN: 1043-1802

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel bilayer-forming phospholipid analog with a photoactivable carbene-generating head group was synthesized and characterized with respect to mol. structure and light-induced reactivity. N'-(1,2-Dimyristoyl-sn-glycero-3-phosphoethyl)-N-[m-[3-(trifluoromethyl)diazirin-3-yl]phenyl]thiourea (PED) was prepared by thiocarbonylation of synthetic dimyristoylphosphatidylethanolamine with 3'-(trifluoromethyl)-3-(m-isothiocyanophenyl)diazirine. PED formed liposomes in aqueous media. Gel to liquid-crystalline transitions occurred at 10.5°. Neither PED- nor PED/dimyristoylphosphatidylcholine mixed liposomes underwent major structural changes when photoactivated. Liposome sizes, determined by electron

microscopy, were not altered upon light exposure. PED combines the advantages of facile synthesis and timed carbene reactivity by photoactivation at wavelengths  $\geq 320$  nm. Conditions used for PED photoactivation did not inactivate catalytically active or complex-forming proteins. Light-induced binding of aqueous-soluble proteins to PED containing liposomes was attained through photoactivation in the presence of myoglobin, streptavidin, or trypsin. The proteins mentioned were utilized to characterize carbene-initiated ligand coupling. Procedures described establish a new and versatile method for the formation of proteoliposomes.

IT 142065-29-QP

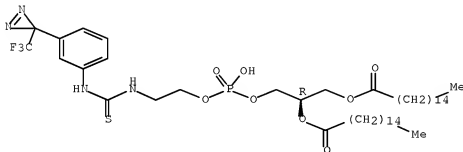
RL: PREP (Preparation)

(preparation of)

RN 142065-29-0 CAPLUS

CN Hexadecanoic acid, 1-[3-hydroxy-3-oxido-8-thioxo-8-[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]-2,4-dioxo-7-aza-3-phosphaoct-1-yl]-1,2-ethanediyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 137043-97-1P

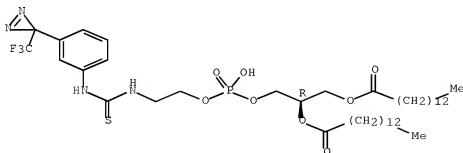
RL: PREP (Preparation)

(preparation of and light-induced coupling of aqueous-soluble proteins to liposomes formed from)

RN 137043-97-1 CAPLUS

CN Tetradecanoic acid, 1-[3-hydroxy-3-oxido-8-thioxo-8-[[3-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]amino]-2,4-dioxo-7-aza-3-phosphaoct-1-yl]-1,2-ethanediyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L8 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1991:626532 CAPLUS Full-text

DOCUMENT NUMBER: 115:226532

ORIGINAL REFERENCE NO.: 115:38494h,38495a

TITLE: Planar bilayer membranes from photoactivable phospholipids

AUTHOR(S): Borle, Francois; Saenger, Michael; Sigrist, Hans  
CORPORATE SOURCE: Inst. Biochem., Univ. Berne, Bern, CH-3012, Switz.  
SOURCE: Biochimica et Biophysica Acta, Biomembranes (1991),  
1066(2), 144-50

CODEN: BBBMBS; ISSN: 0005-2736

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Planar bilayer membranes formed from photoactivable phospholipids have been characterized by low-frequency voltammetry. Cyclic voltammetric measurements were applied for simultaneous registration of planar membrane conductivity and capacitance. The procedure has been utilized to characterize the formation and stability of planar bilayer membranes. Bilayer membranes were formed from N'-(1,2-dimyristoyl-sn-glycero-3-phosphoethyl)-N-(m-3-trifluoromethyldiazirine)phenylthiourea (C14-PED), a head-group photosensitive phospholipid. In situ photoactivation of C14-PED at wavelengths  $\geq 320$  nm altered neither the mean conductivity nor the capacitance of the bilayer. Ionophore (valinomycin) and ion channel (gramicidin) activities were not impaired upon photoactivation. In contrast, bilayer membranes formed from 1,2-bis(hexadeca-2,4-dienoyl)-sn-glycero-3-phosphocholine (C16-DENPC) revealed short life times. In situ photopolymn. of the diene fatty acids significantly increased the membrane conductivity or led to membrane rupture.

IT 137043-97-1

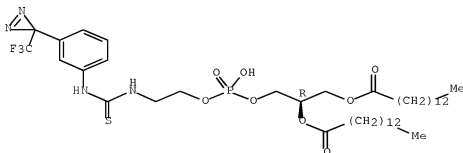
RL: BIOL (Biological study)

(planar bilayer membrane, transport and elec. properties and stability of, photoactivation effect on)

RN 137043-97-1 CAPLUS

CN Tetradecanoic acid, 1-[3-hydroxy-3-oxido-8-thioxo-8-[[3-[3-(trifluoromethyl)-3H-diazirine-3-yl]phenyl]amino]-2,4-dioxo-7-aza-3-phosphaoct-1-yl]-1,2-ethanediyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



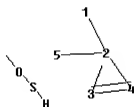
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(7 CITINGS)

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nk

6



chain nodes :

1 5 6 7 8 9 10

ring nodes :

2 3 4

chain bonds :

1-2 2-5 7-8 8-9 9-10

ring bonds :

2-3 2-4 3-4

exact/norm bonds :

2-3 2-4 3-4 7-8 8-9

exact bonds :

1-2 2-5 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:CLASS

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Number of Carbon Atoms : less than 7

6:

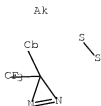
Number of Carbon Atoms : 7 or more

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L9 HAS NO ANSWERS

L9 STR



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L12 0 L10

=> s l11

L13 2 L11

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L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:501975 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 147:136915

TITLE: Convenient Synthesis of Photoaffinity Probes and Evaluation of Their Labeling Abilities

AUTHOR(S): Kan, Toshiyuki; Kita, Yoichi; Morohashi, Yuichi; Tominari, Yusuke; Hosoda, Shinnosuke; Tomita, Taisuke; Natsugari, Hideaki; Iwatsubo, Takeshi; Fukuyama, Tohru  
CORPORATE SOURCE: School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, 422-8526, Japan

SOURCE: Organic Letters (2007), 9(11), 2055-2058

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:136915

AB Convenient synthesis of a variety of photoaffinity probes was accomplished by utilizing the authors' Ns strategy and novel resin. The synthetic probes were evaluated via the labeling ability with the presenilin 1 C-terminal fragments, which was identified as a therapeutic target for Alzheimer's disease.

IT 943601-12-5P

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(convenient synthesis of photoaffinity probes and evaluation of their labeling abilities with presenilin 1 C-terminal fragments as drug targets for Alzheimer's disease)

RN 943601-12-5 CAPLUS

CN Glycinamide, N-[2-(3,5-difluorophenyl)acetyl]-L-alanyl-N-[[2-[[30-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-17,26-dioxo-21,22-dithia-9,18,25-triazatriacont-1-yl]oxy]-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]methyl]-2-phenyl-, (2S)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

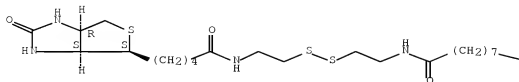
CM 1

CRN 943601-11-4

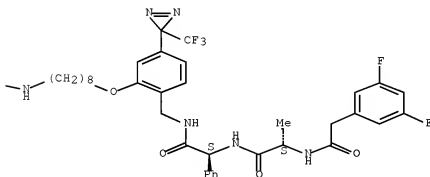
CMF C58 H79 F5 N10 O7 S3

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CM 2

CRN 76-05-1

CMF C2 H F3 O2



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)  
 REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1980:491438 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 93:91438  
 ORIGINAL REFERENCE NO.: 93:14602h,14603a  
 TITLE: Analysis of membranes photolabeled with lipid analogs.

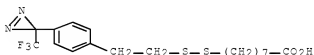


Reaction of phospholipids containing a disulfide group and a nitrene or carbene precursor with lipids and with gramicidin A  
 Brunner, Josef; Richards, Frederic M.  
 Dep. Mol. Biophys. Biochem., Yale Univ., New Haven, CT, 06520, USA  
 Journal of Biological Chemistry (1980), 255(8), 3319-29  
 CODEN: JBCHA3; ISSN: 0021-9258

AUTHOR(S):  
 CORPORATE SOURCE:  
 SOURCE:  
 DOCUMENT TYPE:  
 LANGUAGE:  
 AB

Analogues of fatty acids were synthesized which contain an SS bridge in the aliphatic chain and at the  $\alpha$ -carbon the photoactivatable p-(3-trifluoromethyldiazirino)phenyl or p-azidophenyl group as a carbene and nitrene precursor, resp. These acids were used to acylate 1-palmitoylphosphatidylcholine by the procedure of C. M. Gupta et al. (1977). Multilamellar liposomes prepared from various radioactively labeled lipids and 2-10 mol% of 1 of the photosensitive phospholipid analogs were photolyzed and the extent of crosslinking was determined. The carbene-generating probe labeled dipalmitoylphosphatidylcholine in yields of 15-20%, while labeling with the nitrene probe was approx. 10-fold less efficient. In contrast, these probes were found to react with the unsatd. fatty acid of 1-palmitoyl-2-oleoylphosphatidylcholine with almost equal efficiency. The nitrene was 2-3-fold more efficient than the carbene in crosslinking to gramicidin A. Amino acid anal. and Edman degradation of the labeled peptide indicated that both probes predominantly attacked tryptophan residues. No geometrical correlation was found between the expected penetration of the reactive group of the probe within the bilayer and the labeled sites of the peptide. This result is discussed in terms of chemical selectivities of the photoactivated intermediates. After photocrosslinking, the SS bridge can be cleaved to generate a free SH group which subsequently can be utilized for preparative or anal. purposes. Photolabeled lipids and peptides can be separated easily from the bulk of the unlabeled material. These phospholipid analogs are substrates for the phospholipid exchange protein isolated from calf liver. Transfer from sonicated dispersions of the analogs into an acceptor membrane was demonstrated. Individual monolayers thus can be labeled sep. with these reagents.

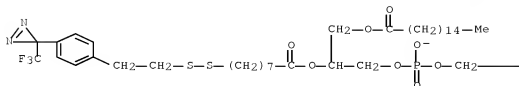
IT 74328-72-6P  
 RL: PREP (Preparation)  
 (preparation of and anhydride formation therefrom)  
 RN 74328-72-6 CAPLUS  
 CN Octanoic acid, 8-[[2-[4-[3-(trifluoromethyl)-3H-diazirin-3-yl]phenyl]ethyl]dithio]- (CA INDEX NAME)



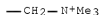
IT 74328-75-9P  
 RL: PREP (Preparation)  
 (preparation of, as membrane probe)  
 RN 74328-75-9 CAPLUS  
 CN 3,5,8-Trioxa-17,18-dithia-4-phosphaeicosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-9-oxo-7-[[[(1-oxohexadecyl)oxy]methyl]-20-[4-[3-

(trifluoromethyl)-3H-diazirin-3-yl]phenyl]-, inner salt, 4-oxide (CA  
INDEX NAME)

PAGE 1-A

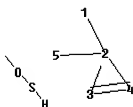


PAGE 1-B



**AK**

**6**



chain nodes :  
1 5 6 7 8 9 10  
ring nodes :  
2 3 4  
chain bonds :  
1-2 2-5 7-8 8-9 9-10  
ring bonds :  
2-3 2-4 3-4  
exact/norm bonds :  
2-3 2-4 3-4 7-8 8-9  
exact bonds :  
1-2 2-5 9-10

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS

Generic attributes :

1:  
Saturation : Unsaturated  
Number of Carbon Atoms : less than 7

6:  
Number of Carbon Atoms : 7 or more

L14        STRUCTURE UPLOADED

=> d l14  
L14 HAS NO ANSWERS  
L14                STR

Ak



Structure attributes must be viewed using SIN Express query preparation.

=> s l14  
SAMPLE SEARCH INITIATED 18:17:11 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED -        2 TO ITERATE

100.0% PROCESSED            2 ITERATIONS            0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                              BATCH    \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:        2 TO        124  
PROJECTED ANSWERS:            0 TO        0

L15            0 SEA SSS SAM L14

=> s l14 full  
FULL SEARCH INITIATED 18:17:20 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED -        54 TO ITERATE

100.0% PROCESSED            54 ITERATIONS            0 ANSWERS  
SEARCH TIME: 00.00.01

L16            0 SEA SSS FUL L14

=> s (aryldiazirine and thiol)  
          0 ARYLDIAZIRINE  
          85189 THIOL  
          26 THIOLS  
          85189 THIOL  
          (THIOL OR THIOLS)  
L17            0 (ARYLDIAZIRINE AND THIOL)

```

=> s (diazirine and thiol)
    1562 DIAZIRINE
    85189 THIOL
    26 THIOLS
    85189 THIOL
        (THIOL OR THIOLS)
L18      4 (DIAZIRINE AND THIOL)

=> s l18
L19      5 L18

=> d hitstr 1-5

L19 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
IT 142438-45-7, 3H-Diazirine-3-thiol
    RL: PRP (Properties)
        (MO calcns. for)
RN 142438-45-7 CAPLUS
CN 3H-Diazirine-3-thiol (CA INDEX NAME)

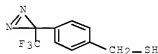
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L19 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
IT 152540-05-1
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (formation of and reaction with dithionitrobenzoic acid)
RN 152540-05-1 CAPLUS
CN Benzenemethanethiol, 4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX NAME)

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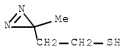
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L19 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
IT 142438-45-7, 3H-Diazirine-3-thiol
    RL: PRP (Properties)
        (isodesmic stabilization energy and isomerization energy of, MO calcn. of)
RN 142438-45-7 CAPLUS
CN 3H-Diazirine-3-thiol (CA INDEX NAME)

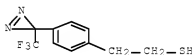
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L19 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2009 ACS on SIN  
 IT 136353-74-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and coupling with bromocyclohexene derivative)  
 RN 136353-74-7 CAPLUS  
 CN 3H-Diazirine-3-ethanethiol, 3-methyl- (CA INDEX NAME)



L19 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2009 ACS on SIN  
 IT 74328-71-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reaction with sulfenylthiocarbonates)  
 RN 74328-71-5 CAPLUS  
 CN Benzeneethanethiol, 4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (CA INDEX  
 NAME)



=> s (diazirine and dextran)  
 1132 DIAZIRINE  
 277 DIAZIRINES  
 1218 DIAZIRINE  
 (DIAZIRINE OR DIAZIRINES)  
 41674 DEXTRAN  
 4436 DEXTRANS  
 42587 DEXTRAN  
 (DEXTRAN OR DEXTRANS)  
 L20 4 (DIAZIRINE AND DEXTRAN)

=> d hitstr 1-4

L20 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on SIN

L20 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN  
 L20 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN  
 L20 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN

=> d ibib abs hitstr L20 1-4

L20 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2005:1304564 CAPLUS Full-text  
 DOCUMENT NUMBER: 144:33834  
 TITLE: Dextran-coated surface for sensors  
 INVENTOR(S): Barie, Nicole; Gobet, Jean; Rapp, Michael; Sigrist,  
 Hans  
 PATENT ASSIGNEE(S): Forschungszentrum Karlsruhe GmbH, Germany; Centre  
 Suisse d'Electronique et de Microtechnique S.A.  
 SOURCE: U.S., 8 pp., Cont.-in-part of Appl. No.  
 PCT/EP99/02599.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6974707	B1	20051213	US 2000-694241	20001023
DE 19818360	A1	19991104	DE 1998-19818360	19980424
DE 19818360	C2	20000531		
WO 9956119	A1	19991104	WO 1999-EP2599	19990419
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:		DE 1998-19818360 A 19980424 WO 1999-EP2599 A2 19990419		

AB A dextran-coated carrier having a surface with a connection between dextran disposed as coating on the carrier formed by a photolinker, said dextran coating being formed on and covalently attached to said carrier by co-immobilization resulting from a mixture of the dextran and a 3-trifluoromethyl-3-(m-isothiocyanophenyl) diazine (TRIMID) modified aminodextran, wherein the dextran is attached to the carrier through a component resulting from the irradiation of the 3-trifluoromethyl-3-(m-isothiocyanophenyl) diazine (TRIMID) modified aminodextran.  
 OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
 (4 CITINGS)  
 REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2005:493757 CAPLUS Full-text  
 DOCUMENT NUMBER: 143:22656  
 TITLE: Photolinker macromolecules, metallic substrates,  
 ligands modified with the linkers, and process of  
 preparation  
 INVENTOR(S): Sigrist, Hans; Chai Gao, Hui; Soury-Lavergne, Isabelle  
 PATENT ASSIGNEE(S): C.S.E.M. Centre Suisse d'Electronique et de  
 Microtechnique, Swiss.  
 SOURCE: PCT Int. Appl., 28 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent

LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005052580	A1	20050609	WO 2004-CH704	20041123
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1563306	A1	20050817	EP 2004-797261	20041123
EP 1563306	B1	20070214		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR, IS, YU				
US 20070149775	A1	20070628	US 2006-580317	20060523
PRIORITY APPLN. INFO.: EP 2003-405851 A 20031128 WO 2004-CH704 W 20041123				

AB The invention relates to a photolinker macromol. comprising photoactivable groups and sulfur-containing groups, which is attached to a metallic substrate, and optionally covalently bonded to a ligand, and the use thereof in biosensor systems, microarrays, nanoparticles, nanoassemblies and microparticles useful in bioanalytics, or the pharmaceutical, or textile industry. Thus OptoDex S was synthesized starting from aminodextran and 3-(trifluoromethyl)-3-(m-isothiocyanophenyl) diazirine; the obtained OptoDex A was treated on a chromatog. column with sulfosuccinimidyl-6-[3'-(2-pyrimidylidithio)propionamido] hexanoate (LC sulfo SPDP). OptoDex S was chemisorbed onto gold surfaces; fluorophor (Cy5)-labeled riboflavin binding protein, Cy3-labeled BSU and non-labeled mouse Ig were photoimmobilized to the OptoDex S-gold surface. Vitamin B2 was determined by surface plasmon resonance using the photoimmobilized riboflavin binding protein surface.

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2005:182876 CAPLUS Full-text  
 DOCUMENT NUMBER: 142:263005  
 TITLE: Methods of chemical and biochemical functionalization of yarn and textile products  
 INVENTOR(S): Sgrist, Hans; Crevoisier, Francois; Chai, Gao Hui  
 PATENT ASSIGNEE(S): Csem Centre Suisse D'electronique Et De Microtechnique Sa, Switz.  
 SOURCE: PCT Int. Appl., 41 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005019518 A1 20050303 WO 2004-IB2962 20040826  
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
EP 1664416 A1 20060607 EP 2004-769354 20040826  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK  
US 20070026239 A1 20070201 US 2006-569510 20060724  
PRIORITY APPLN. INFO.: GB 2003-19929 A 20030826  
WO 2004-IB2962 W 20040826

AB Methods of chemical and biochem. functionalization of yarn and textile products are described. A yarn or textile product is contacted with a linker mol. comprising two or more photochem. activatable chemical groups and a non-linker mol. having a desired property. Photochem. activation of the chemical groups causes covalent attachment of the non-linker mol. to the yarn or textile product by means of the linker mol. in a single step. The methods are particularly useful for immobilization to yarn or textile of biomols. that are susceptible to denaturation. Use of linker mols. derived from proteins or polysaccharides further minimizes denaturation of the biomol.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1996:174574 CAPLUS Full-text  
DOCUMENT NUMBER: 124:223317  
ORIGINAL REFERENCE NO.: 124:41185a,41188a

TITLE: Pore formation by *S. aureus*  $\alpha$ -toxin in liposomes and planar lipid bilayers: effects of nonelectrolytes  
AUTHOR(S): Bashford, C. L.; Alder, G. M.; Fulford, L. G.; Korchev, Y. E.; Kovacs, E.; MacKinnon, A.; Pederzoli, C.; Pasternak, C. A.

CORPORATE SOURCE: Div. Biochemistry, St. George's Hosp. Med. Sch., London, SW17 0RE, UK

SOURCE: Journal of Membrane Biology (1996), 150(1), 37-45  
CODEN: JMBBBO; ISSN: 0022-2631

PUBLISHER: Springer  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Nonelectrolytes such as polyethylene glycols (PEG) and dextrans (i) promote the association of *S. aureus*  $\alpha$ -toxin with liposomes (shown by Coomassie staining) and (ii) enhance the rate and extent of calcein leakage from calcein-loaded liposomes; such leakage is inhibited by  $H^+$ ,  $Zn^{2+}$  and  $Ca^{2+}$  to the same extent as that of nonPEG-treated liposomes. Incubation of liposomes treated with  $\alpha$ -toxin in the presence of PEG with the hydrophobic photo-affinity probe 3-(trifluoromethyl)-3-m-([125I]iodophenyl)diazirine(125I-TID) labels monomeric and-predominantly-hexameric forms of liposome-associated  $\alpha$ -toxin; in the absence of PEG little labeling is apparent. At high concns. of  $H^+$  and  $Zn^{2+}$  but not of  $Ca^{2+}$ -all of which inhibit calcein leakage-the distribution of label between hexamer and monomer is perturbed in favor of the latter. In  $\alpha$ -toxin-treated planar lipid bilayers from which excess toxin has been washed away, PEGs and dextrans strongly promote the appearance of ion-conducting pores. The properties of such pores are similar in most regards to



pores induced in the absence of nonelectrolytes; they differ only in being more sensitive to "closure" by voltage (as are pores induced in cells). In both systems, the stimulation by nonelectrolytes increased with concentration and with mol. mass up to a maximum around 2,000 Da. The authors conclude (i) that most of the  $\alpha$  toxin that becomes associated with liposome or planar lipid bilayers does not form active pores and (ii) that the properties of  $\alpha$ -toxin-induced pores in lipid bilayers can be modulated to resemble those in cells.

OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS  
RECORD (13 CITINGS)